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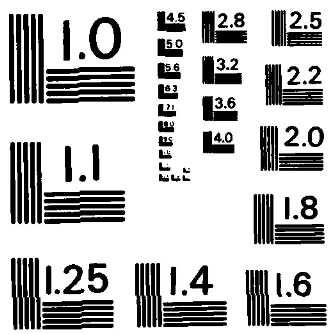

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ORDERING METHODS FOR SPARSE MATRICES: ANNUAL REPORT

AFOSR Contract F49620-81-0072

Report No. 1

Annual Report for the Period

July 1, 1981 - June 30, 1982

by

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Boeing Computer Services Company

August 20, 1982

KEY WORDS AND PHRASES: linear equations, sparse matrices, reordering algorithms, Hellerman-Rarick algorithm, P4 algorithm, unsymmetric matrices, Gauss elimination.

ABSTRACT: This report summarizes the activities at Boeing Computer Services Company on AFOSR Contract F49620-81-C-0072 from July 1, 1981 until June 30, 1982. Five tasks are defined: creation of a comprehensive test matrix collection, analysis of the Hellerman-Rarick P4 algorithm, production of a P4 code, production of a diagnostic code, and comparative analysis of several algorithms using the test matrices and the diagnostic code. Status reports on the five tasks are given, relevant reports and publications of project personnel are listed and related sparse matrix activities are discussed. Work is progressing well on the project. Several promising and stable variations of the Hellerman-Rarick algorithm have been found and will be thoroughly tested in the next phase of the project.

INTRODUCTION

The solution of systems of large sparse linear equations is a fundamental computational step in the numerical solution of many scientific and engineering problems. These problems arise in such diverse areas as structural analysis, linear programming, network analysis, chemical process design, electromagnetic pulse (EMP) analysis, optimization, steady state analysis, and policy planning. When direct solution methods are used to solve these equations one of the major difficulties is choosing a reordering of the rows and columns of the sparse matrix to reduce some measure of solution cost.

Because sparse matrix research has grown independently out of many disciplines, there are many different heuristic methods (band, profile, Markowitz, tearing, P4, and variations) presently used to accomplish this reordering. The challenge in building standard software is to determine if one heuristic works adequately across a broad class of problems, or if several heuristics must be available in a general purpose code. If several heuristics are needed, matrix classes must be identified as a basis for matching a given matrix with the proper ordering method. In either case it also must be determined how much performance will improve for particular problem classes if specialized sparse matrix code rather than general purpose code is used.

This research project is concerned with answering these questions. This report describes the current status of the project. The following topics are covered by this report: research objectives, status of the research effort, relevant publications by the project personnel, professional personnel associated with the research effort, and related sparse matrix activities at Boeing Computer Services.

RESEARCH OBJECTIVES

The research objectives have been broken down into five tasks.

<u>Task 1: Creation of a Comprehensive Test Matrix Collection.</u> The goal of this task is to assemble a large collection of sparse matrices. These matrices will be representative of realistic problems arising in many different application areas. They should be of varying sizes and structural characteristics. Considerable effort is going into this task in order to have a comprehensive collection.

<u>Task 2: Analyze the Hellerman-Rarick P4 Algorithm.</u> In this task the Hellerman-Rarick reordering algorithm for sparse unsymmetric linear equations and all of its known variations will be studied with the intent of understanding the applicability, stability, and effectiveness of it. A precise algorithmic description of the most important version will be produced. This description will form the basis for studying the different variations.

Task 3: Producing a P4 Code. The precise algorithic description of the Hellerman-Rarick algorithm from Task 2 will be used to produce a high quality FORTRAN code implementing the algorithm. This code will include all modifications which are improvements of the original algorithm.

Task 4: Producing a Diagnostic Code. A diagnostic program will be produced which will be capable of monitoring the effectiveness of various ordering algorithms applied to sparse matrices. The diagnostic code will monitor many characteristics such as accuracy, fill-in, storage, run time and operation counts.

Task 5: Comparative Analysis. This final task is to utilize the test collection (Task 1) and the diagnostic program (Task 4) to provide detailed comparisons of various ordering algorithms including the Hellerman-Rarick algorithm (Task 3) and the MA28 code from the Harwell library.

STATUS OF THE RESEARCH EFFORT

The project is progressing as planned. Tasks 2 and 4 have been completed during the first year of this project. Task 1 is continuing into the second year of the project. Task 3 is now underway and Task 5 will start in late summer of 1982 and continue through the winter of 1982-1983. This section describes those activities.

Task 1. We have contacted many people from different application areas who have sparse matrix problems and we have asked that certain of the matrices be sent to us. Test problems from structural engineering, chemical process design, linear programming, circuit analysis and optimization have been identified. We have received some of the test matrices and expect to continue receiving the matrix collections for several more months. We have published a request for test matrices in the ACM SIGNUM Newsletter and in the IMANA Newsletter. We have recruited test problems at recent professional meetings including the SIAM Conference on Applied Linear Algebra and the SIAM 30th Anniversary Meeting. This task is being performed in collaboration with Dr. Iain Duff of AERE Harwell in England.

Task 2. We have analyzed the Hellerman-Rarick P4 algorithm and have produced a very simple algorithmic des[illegible]on of it. Previous descriptions have been rather lengthy and complicated [illegible] thus, have made analysis difficult. Our simplified description has led t[illegible] understanding of how the algorithm works and what types of problems cause it difficulties. Because of the simplified description, we also have been able to analyze modifications of the algorithm. Several modifications seem very promising. In fact, they cannot break down because of intermediate structural singularity, a problem with other versions of the Hellerman-Rarick algorithm. This work was discussed at the SIAM Meeting at Stanford University, July 19-23, 1982. These modifications will be tested for their effectiveness on the test matrix collection in Task 5.

Task 3. We have two different existing Hellerman-Rarick P4 codes: one from Mike Saunders of Stanford University and one from the World Bank. We have converted both of these codes so that they can interact with our diagnostic code (task 4). We are also in the process of incorporating our modifications into those codes. When that is completed we will be ready to begin our comprehensive testing work.

Task 4. The diagnostic program has been designed, written, and tested. It collects and analyzes data concerning the performance of the different ordering algorithms. This information will be instrumental in deciding which algorithms are most effective for various matrix problems in our collection of test matrices. The types of data to be gathered include order of the matrix, number of nonzeros in different parts of the matrix, nearness to symmetry, storage required fill-in, execution times, operation counts, stability bounds and relative density. The diagnostic program measures the ordering algorithm's ability in reducing the amount of computer memory required to store the factored matrix as well as reducing the number of operations for the actual factorization. This program will be used to monitor the results of the algorithms tested in task 5.

Task 5. This task is just now starting and will be the major focus of the remainder of the contract work.

RECENT RELEVANT REPORTS AND PUBLICATIONS OF THE PROJECT PERSONNEL

David S. Dodson and Roger G. Grimes, "Remark on Algorithm 539," to appear in ACM Transactions on Mathematical Software.

Iain S. Duff, Roger G. Grimes, John G. Lewis and William G. Poole, Jr., "Sparse Matrix Test Problems," ACM SIGNUM Newsletter, Volume 17, No. 2, June 1982, page 22, and IMANA Newsletter, Volume 6, No. 3, April 1982, page 19.

A. M. Erisman, "Sparse Matrix Problems in Electric Power System Analysis," in Sparse Matrices and their Uses, Iain S. Duff, editor, Academic Press, New York, 1981.

Roger G. Grimes and John G. Lewis, "Condition Number Estimation for Sparse Matrices," SIAM Journal on Scientific and Statistical Computing, Volume 2, No. 4, December 1981, pages 384-388.

John G. Lewis, "ALGORITHM 582: The Gibbs-Poole-Stockmeyer and Gibbs-King Algorithms for Reordering Sparse Matrices," ACM Transactions on Mathematical Software, Vol. 8, No. 2, June 1982, pages 190-194.

John G. Lewis, "Implementation of the Gibbs-Poole-Stockmeyer and Gibbs-King Algorithms," ACM Transactions on Mathematical Software, Vol. 8, No. 2, June 1982, pages 180-189.

John G. Lewis, "Remark on Algorithms 508 and 509," ACM Transactions on Mathematical Software, Vol. 8, No. 2, June 1982, page 221.

John G. Lewis and William G. Poole, Jr., "Ordering Algorithms Applied to Sparse Matrices in Electric Power Problems," in Electric Power Problems: The Mathematical Challenge, A. M. Erisman, K. W. Neves and M. H. Dwarakanath, editors, SIAM, Philadelphia, 1980.

RECENT ABSTRACTS PREPARED FOR PRESENTATION AT PROFESSIONAL MEETINGS

The following abstracts are preliminary reports of work in progress. It is expected that several papers will result from our work during the next year.

Iain S. Duff, Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., "Sparse Matrix Test Problems," to be presented at the Sparse Matrix Symposium 1982, Fairfield Glade, Tennessee, October 25-27, 1982.

Albert M. Erisman, "Matrix Modification and Partitioning," to be presented at the Sparse Matrix Symposium 1982, Fairfield Glade, Tennessee, October 25-27, 1982.

Albert M. Erisman, Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., "The Hellerman-Rarick P4 Algorithm for Reordering Unsymmetric Sparse Matrices. Part I: The Algorithm," presented at the SIAM 30th Anniversary Meeting, Stanford University, Stanford, California, July 19-23, 1982.

Albert M. Erisman, Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., "The Hellerman-Rarick P4 Algorithm for Reordering Unsymmetric Sparse Matrices. Part II: Structural Singularity and Modifications," presented at the SIAM 30th Anniversary Meeting, Stanford University, Stanford, California, July 19-23, 1982.

Albert M. Erisman, Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., "A Structurally Stable Modification of the Hellerman-Rarick Algorithm for Reordering Unsymmetric Sparse Matrices," to be presented at the Sparse Matrix Symposium 1982, Fairfield Glade, Tennessee, October 25-27, 1982.

Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., "Program for the Comparison of Reordering Algorithms for the Solution of Unsymmetric Sparse Systems of Equations," to be presented at the Sparse Matrix Symposium 1982, Fairfield Glade, Tennessee, October 25-27, 1982.

PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

Four people from Boeing Computer Services, Albert M. Erisman, Roger G. Grimes, John G. Lewis, and William G. Poole, Jr., have performed almost all of the work of this project. Task 1, which is concerned with the creation of a comprehensive test matrix collection, is being carried out in collaboration with Dr. Iain S. Duff of AERE, Harwell, England.

RELATED SPARSE MATRIX ACTIVITIES AT BOEING COMPUTER SERVICES COMPANY

The mathematicians at Boeing Computer Services working on this project also are active in other projects which involve sparse matrix computations. This section briefly describes some of the most recent activities by those people. These projects are not funded by the AFOSR contract but they indicate the significant role that sparse matrix research plays at BCS.

<u>Sparse Matrix Computations in Electric Power Problems.</u> A. M. Erisman, R. G. Grimes, J. G. Lewis and W. G. Poole, Jr. have performed work recently which applied current sparse matrix technology to electric power problems. Two recently completed publications in this area are included in the earlier section on reports and publications. They appeared in the proceedings of two conferences: the SIAM meeting on <u>Electric Power Problems: The Mathematical Challenge</u> and the IMA conference on <u>Sparse Matrices and their Uses</u>.

<u>Condition Number Estimation for Sparse Matrices.</u> R. G. Grimes and J. G. Lewis have defined and implemented a condition number estimator for sparse matrices. The estimator has been implemented in a large, sparse eigenvalue program. A paper in the <u>SIAM Journal on Scientific and Statistical Computing</u> is mentioned in the section on publications.

<u>Band and Envelope Reordering for Sparse Matrices.</u> J. G. Lewis has greatly improved the Gibbs-Poole-Stockmeyer and Gibbs-King algorithm implementations for reducing the bandwidth and profile of a symmetric sparse matriix. Two papers and a short remark recently appeared in <u>ACM Transactions on Mathematical Software</u> (see section on publications).

<u>Sparse Vector and Matrix Building Blocks for the CRAY-1.</u> All four of the mathematicians on this project have been involved in developing, implementing and testing assembler language basic building blocks for sparse vector and matrix computations on the CRAY-1 computer. These subprograms are a part of CRAYPACK.

<u>CRAY-1 Optimization of SPARSPAK and COMPLEX version of SPARSPAK.</u> Several people at Boeing Computer Services have modified SPARSPAK so that a version optimized for the CRAY-1 and a COMPLEX version have been produced.

Problems from Structural Engineering. J. G. Lewis has tested several problems from structural engineering by exercising the various ordering algorithms in SPARSPAK. The preliminary results indicate that no single ordering algorithm will suffice for a general code. A Lanczos-based eigenvalue solver has also been developed for structural engineering codes. A version for the CRAY-1 computer has been prepared.

The Necessity of Pivoting. W. Kahan (of the University of California, Berkeley) and W. G. Poole, Jr. are working on a paper which discusses the conditions under which matrices do not need some form of pivoting for maintaining numerical stability.

SIAM Conference on Applied Linear Algebra. J. G. Lewis attended this conference in Raleigh, North Carolina in April 1982. At the conference, he publicized the sparse matrix collection and requested sample problems.

Sparse Matrix Symposium 1982. W. G. Poole, Jr. is a member of the Advisory Committee for this symposium. A. M. Erisman, R. G. Grimes, and J. G. Lewis also plan to attend and present papers.

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFOSR-TR- 82-0932	2. GOVT ACCESSION NO. A121306	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) ORDERING METHODS FOR SPARSE MATRICES		5. TYPE OF REPORT & PERIOD COVERED INTERIM, 1 JUL 81-30 JUN 82
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) William G. Poole, Jr.		8. CONTRACT OR GRANT NUMBER(s) F49620-81-C-0072
9. PERFORMING ORGANIZATION NAME AND ADDRESS Energy Technology Applications Division, Boeing Computer Services Company, MS 9C-01, 565 Andover Park West, Tukwila WA 98188		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS PE61102F; 2304/A3
11. CONTROLLING OFFICE NAME AND ADDRESS Directorate of Mathematical & Information Sciences Air Force Office of Scientific Research Bolling AFB DC 20332		12. REPORT DATE 20 AUG 1982
		13. NUMBER OF PAGES 7
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION ST. MENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY TES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Sparse matrices; reordering algorithms; Hellerman-Rarick; P4; unsymmetric matrices; Gauss elimination.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report summarizes the activities at Boeing Computer Services Company on AFOSR Contract F49620-81-C-0072 from 1 July 1981 until 30 June 1982. Five tasks are defined: creation of a comprehensive test matrix collection, analysis of the Hellerman-Rarick P4 algorithm, production of a P4 code, production of a diagnostic code, and comparative analysis of several algorithms using the test matrices and the diagnostic code. Status reports on the five tasks are given, relevant reports and publications of project personnel are listed and related sparse matrix activities are discussed. Work is progressing well. (CONTINUED)

ITEM #20, CONTINUED: on the project. A very promising and stable variation of the Hellerman-Rarick algorithm has been found and will be tested in the next phase of the project.